

New quantum-mechanical phenomenon in a model of electron-electron interaction in graphene.

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A quantum mechanical model of two interacting electrons in graphene is considered. We concentrate on the case of zero total momentum of the pair. We show that the dynamics of the system is very unusual. Both stationary and time-dependent problems are considered. It is shown that the complete set of the wave functions with definite energy includes the new functions, previously overlooked. The time evolution of the wave packet, corresponding to the scattering problem setup, leads to the appearance of the localized state at large time. The asymptotics of this state is found analytically. We obtain the lower bound of the life time of this state, which is connected with the breakdown of the continuous model on the lattice scale. The estimate of this bound gives one a hope to observe the localized states in the experiment.

PACS numbers: 73.20.Mf, 73.22.Pr, 03.65.Ge, 03.65.Nk

I. INTRODUCTION

Nowadays a great deal of effort has been devoted to the experimental investigation of the transport properties of graphene, see recent review¹. One of the important results of these experiments is the observation of high mobility of the charge carriers². Many papers have been devoted to the investigation of the influence of the electron-impurity interaction on the mobility of the charge carriers, see reviews^{3,4}. Study of the electron-electron interaction in graphene is also important for understanding of this effect, see Ref.⁵. However, a theoretical progress in this problem is rather limited^{3,4}.

It is well established now that the low-energy single electron dynamics in graphene is described by a massless two-component Dirac equation^{2,6-9}

$$i\hbar\partial_t\psi(t, \mathbf{r}) = \hat{h}\psi(t, \mathbf{r}),$$

where the hamiltonian \hat{h} has the form

$$\hat{h} = v_F \boldsymbol{\sigma} \cdot \hat{\mathbf{p}},$$

v_F is the Fermi velocity, $\hat{\mathbf{p}} = -i\hbar\nabla$, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the Pauli matrices acting on the pseudospin variables. Below we set $\hbar = v_F = 1$. Evidently, the pair of non-interacting electrons can be described by the equation

$$i\partial_t\psi(\mathbf{r}_1, \mathbf{r}_2, t) = \hat{H}_0\psi(\mathbf{r}_1, \mathbf{r}_2, t), \quad (1)$$

$$\hat{H}_0 = \hat{h}_1 + \hat{h}_2 = \boldsymbol{\sigma}_1 \cdot \hat{\mathbf{p}}_1 + \boldsymbol{\sigma}_2 \cdot \hat{\mathbf{p}}_2, \quad (2)$$

where $\psi(\mathbf{r}_1, \mathbf{r}_2, t)$ is the wave function of the system, depending on the coordinates and pseudospin variables of both electrons. The generalization of Eq. (1) to the case of interacting electrons is a highly nontrivial problem. The origin of the difficulties is the necessity to take into account the interaction with the electrons below Fermi surface. This interaction results in the existence of the electron-hole excitations in the intermediate states. The account of the corresponding effects

in quantum electrodynamics (QED) leads to the Dyson-Schwinger equation (which, for the bound states, reduces to the Bethe-Salpeter equation), see, e.g., Ref.¹⁰. However, in the nonrelativistic QED systems, the effect of virtual electron-positron pair in the intermediate states is small. For massless electrons in graphene, the nonrelativistic approximation is not applicable and the effect of virtual electron-hole excitation may be crucially important for the problem of electron-electron interaction. The approach based on the Bethe-Salpeter equation was used in Ref.¹¹ in the investigation of electron-hole interaction in graphene.

Though the influence of the electron-hole excitations can be very important, nevertheless, as a first step in the investigation of the electron-electron interaction, it makes sense to ignore this effect and to model the electron-electron interaction by replacing $\hat{H}_0 \rightarrow \hat{H}_V$ in Eq. (1), where

$$\hat{H}_V = \hat{H}_0 + V(r) = \boldsymbol{\sigma}_1 \cdot \hat{\mathbf{p}}_1 + \boldsymbol{\sigma}_2 \cdot \hat{\mathbf{p}}_2 + V(r) \quad (3)$$

and $V(r) = V(|\mathbf{r}_1 - \mathbf{r}_2|)$ is the electron-electron interaction potential. Recently, this model has been considered in Ref.¹², where the eigenfunctions of \hat{H}_V have been analysed. The solutions found in Ref.¹² appeared to have unusual properties. In order to understand the origin of these properties, we revisit in the present paper the solution of the stationary equation $\hat{H}_V\psi = E\psi$. We also consider the time-dependent problem and demonstrate that the unusual properties of the eigenfunctions of the hamiltonian are reflected in the very specific properties of the time evolution of the wave packets.

We restrict our consideration to the specific case of zero total momentum of the pair and search for the solutions being the eigenstates of the operator

$$\hat{J}^z = \frac{1}{2}(\sigma_1^z + \sigma_2^z) - i\partial_\varphi,$$

where φ is the azimuth angle of the vector $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. We assume that the potential $V(r)$ is a smooth positive

monotonically decreasing vanishing function. To include the important case of the Coulomb potential into the consideration, we allow for the r^{-1} growth of the potential at $r \rightarrow 0$. The solution of the stationary equation shows that the wave functions with $J^z = 0$ are smooth functions for any energy E . This is also valid for the wave functions with $J_z \neq 0$ and the energy above the maximum of the potential $V_{\max} = V(0)$ or below zero. For $J_z \neq 0$ and $0 < E < V_{\max}$, the solution of the stationary equation necessarily has singularity at the point $r_*(E)$ determined by the condition

$$E = V(r_*), \quad (4)$$

which is in agreement with Ref.¹². Such a behaviour contradicts a common wisdom which tells one that the wave function should be a smooth function in the region where the potential is also smooth. We show that the existence of the singularity in the wave function is related to the degeneracy of the derivative matrix in the hamiltonian. We find an important new feature of the energy spectrum: the additional degeneracy of the states with fixed $J^z \neq 0$ and energy in the interval $(0, V_{\max})$.

For the time-dependent problem we choose the initial conditions corresponding to the wide spherical wave packet with fixed J^z and the average energy E_0 (average value of the hamiltonian) moving toward the origin from the large distance $r_0 \gg \Delta$, where Δ is the width of the packet (the energy dispersion in the packet $\sim \Delta^{-1}$). The direct numerical calculation reveals a remarkable picture. At rather large time $t \gtrsim r_0$ one observes not only a reflected wave packet moving toward the large r , but also a narrow peak in the vicinity of $r_*(E_0)$ with the width $\propto 1/\Delta$. The total norm of the wave function is conserved as it should be for a hermitian hamiltonian. In order to check consistency of the results obtained, we demonstrate that the solution of the time-dependent equation based on the decomposition of the initial wave packet over the stationary wave functions reproduces the direct numerical solution of this equation. Using this decomposition, we find the large-time asymptotics of the emerged peak analytically.

II. GENERAL PROPERTIES OF THE MODEL

Obviously, the hamiltonian \hat{H} in Eq. (3) commutes with the total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$, and we can search the wave function in the form $\psi(\mathbf{r}_1, \mathbf{r}_2, t) = \exp(i\mathbf{P}_0 \cdot \mathbf{R}) \psi(t, \mathbf{r})$, where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ is the center-of-energy coordinate and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative position vector. Note that the wave function $\psi(t, \mathbf{r})$ depends nontrivially on the system total momentum \mathbf{P}_0 , see Ref.¹². Below we consider a specific case $\mathbf{P}_0 = 0$. Then the wave equation has the form

$$i\partial_t \psi(t, \mathbf{r}) = \hat{H} \psi(t, \mathbf{r}), \quad (5)$$

$$\hat{H} = (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \hat{\mathbf{p}} + V(r), \quad (6)$$

where $\hat{\mathbf{p}} = -i\nabla$. The hamiltonian \hat{H} commutes with the operator

$$\hat{J}^z = \hat{S}^z + \hat{L}^z = \frac{1}{2}(\sigma_1^z + \sigma_2^z) - i\partial_\varphi \quad (7)$$

(φ is the azimuthal angle of the vector \mathbf{r}) and the operator

$$\hat{O} = \hat{\mathbf{S}}^2 - 2(\hat{S}^z)^2, \quad (8)$$

where $\hat{\mathbf{S}}^2 = \frac{1}{4} \sum_{i=1}^3 (\sigma_1^i + \sigma_2^i)^2$. The operators \hat{J}^z and \hat{O} also commute with each other. Therefore, we can search for the solution of Eq. (5) to be the eigenfunction of \hat{J}^z and \hat{O} :

$$\begin{aligned} \psi_0(t, \mathbf{r}) = e^{iM\varphi} & \left(a_{00}(t, r) |0, 0\rangle + e^{-i\varphi} a_{11}(t, r) |1, 1\rangle \right. \\ & \left. + e^{i\varphi} a_{1-1}(t, r) |1, -1\rangle \right), \end{aligned} \quad (9)$$

$$\psi_2(t, \mathbf{r}) = e^{iM\varphi} g(t, r) |1, 0\rangle \quad (10)$$

so that $\hat{J}^z \psi_k = M \psi_k$ and $\hat{O} \psi_k = k \psi_k$. Here $|s, s_z\rangle$ is the eigenfunction of the operators $\hat{\mathbf{S}}^2$ and \hat{S}^z . It is convenient to pass from the functions a_{ij} to the functions

$$f = i \frac{a_{11} + a_{1-1}}{\sqrt{2}}, \quad h = i \frac{a_{11} - a_{1-1}}{\sqrt{2}}, \quad d = a_{00}. \quad (11)$$

Using Eqs. (5), (9), (10), and (11), we obtain

$$i\partial_t g = V(r) g, \quad (12)$$

$$i\partial_t f = V(r) f - \frac{2M}{r} d, \quad (13)$$

$$i\partial_t h = V(r) h - 2\partial_r d, \quad (14)$$

$$i\partial_t d = V(r) d - \frac{2M}{r} f + 2 \left(\partial_r + \frac{1}{r} \right) h, \quad (15)$$

The last three equations can be represented in the matrix form

$$i\partial_t F = \hat{H}_r F, \quad (16)$$

where

$$F = \begin{pmatrix} f \\ h \\ d \end{pmatrix}, \quad \hat{H}_r = \begin{pmatrix} V(r) & 0 & -\frac{2M}{r} \\ 0 & V(r) & -2\partial_r \\ -\frac{2M}{r} & 2(\partial_r + \frac{1}{r}) & V(r) \end{pmatrix}. \quad (17)$$

It is easy to see that \hat{H}_r is a hermitian operator, i.e.

$$\int_0^\infty dr r F_1^\dagger \hat{H}_r F_2 = \int_0^\infty dr r \left(\hat{H}_r F_1 \right)^\dagger F_2$$

for continuous functions $F_{1,2}(r)$, decreasing sufficiently fast when $r \rightarrow \infty$ and finite at $r = 0$.

The general solution of Eq. (12) is

$$g(t, r) = g(0, r) e^{-iV(r)t}, \quad (18)$$

whereas the general solution of Eq. (16) can not be found analytically.

Conserved current and density. The conserved current and density for Eq. (5) have the form

$$\mathbf{j} = \psi^\dagger (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \psi, \quad \rho = \psi^\dagger \psi. \quad (19)$$

For two solutions ψ_0 and ψ_2 , Eq. (10), the current and density are expressed as

$$\begin{aligned} \psi_0: \quad j_r &= 4 \operatorname{Im}(dh^*), \quad j_\varphi = -4 \operatorname{Re}(df^*), \\ \rho &= |f|^2 + |h|^2 + |d|^2, \end{aligned} \quad (20)$$

$$\psi_2: \quad j_r = 0, \quad j_\varphi = 0, \quad \rho = |g|^2, \quad (21)$$

where j_r and j_φ are the radial and angular components of the current, respectively.

III. STATIONARY PROBLEM

Let us first consider the stationary equation for the function g :

$$Eg = V(r)g. \quad (22)$$

This simple consideration helps one to understand better the properties of the solutions of the stationary equation for the function F . For $E > V_{\max}$, the equation (22) has no solutions, while for $0 < E < V_{\max}$ its formal solution is $g_a(r) = \delta(r - a)$, where a is determined by the equation $E = V(a)$. The functions $g_a(r)$ for different values of a are mutually orthogonal and normalized by the condition

$$\int_0^\infty dr r g_a(r) g_{\tilde{a}}(r) = a \delta(a - \tilde{a}). \quad (23)$$

Note that the density $\rho(r) = |g_a(r)|^2$, Eq. (21), corresponding to this solution, is not well-defined. Nevertheless, the functions $g_a(r)$ form a complete set and can be used to solve the time-dependent problem. Indeed,

$$g(t, r) = \int_0^\infty da e^{-iV(a)t} g(0, a) g_a(r) = g(0, r) e^{-iV(r)t}$$

in agreement with Eq. (18).

Let us now pass to the consideration of the stationary equation

$$EF = \hat{H}_r F. \quad (24)$$

The hamiltonian \hat{H}_r is a first-order differential operator, see Eq. (17). It is known from the theory of ordinary differential equations that the solution y of the system $\partial_r y(r) = A(r) y(r)$ can have singularities only in the points where the elements of the matrix $A(r)$ are singular. We can not, however, represent Eq. (24) in this form

since the matrix $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2 \\ 0 & 2 & 0 \end{pmatrix}$ in front of the derivative ∂_r

in \hat{H}_r is degenerate. We show below that this degeneracy leads, for $M \neq 0$, to the appearance of the singularity of the solution F in the point $r = r_*$.

Second-order equation for d . The explicit form of Eq. (24) reads

$$(E - V) f = -\frac{2M}{r} d, \quad (25)$$

$$(E - V) h = -2\partial_r d, \quad (26)$$

$$(E - V) d = 2\partial_r h + \frac{2}{r} h - \frac{2M}{r} f. \quad (27)$$

Using the first two equations in order to eliminate the functions f and h from the last equation, we obtain

$$d'' + p(r) d' + q(r) d = 0, \quad (28)$$

$$p(r) = \frac{V'}{E - V} + \frac{1}{r}, \quad (29)$$

$$q(r) = \frac{1}{4} (E - V)^2 - \frac{M^2}{r^2}, \quad (30)$$

where a prime denotes the derivative with respect to r .

Boundary condition at $r = 0$. Let us determine the boundary condition at $r = 0$. If $V(0) < \infty$, the general solution of Eq. (28) behaves near $r = 0$ as

$$d \approx a_1 r^{|M|} + a_2 \times \begin{cases} r^{-|M|}, & M \neq 0 \\ \ln r, & M = 0 \end{cases}, \quad (31)$$

while for the case of Coulomb singularity, when $V(r) \xrightarrow{r \rightarrow 0} \alpha/r$, the asymptotics of the general solution has the form

$$d \approx a_1 r^{\nu-1/2} + a_2 r^{-\nu-1/2}, \quad (32)$$

where $\nu = \frac{1}{2} \sqrt{4M^2 + 1 - \alpha^2}$. Here a_1 and a_2 are some constants. We choose the boundary condition at $r = 0$ as

$$a_2 = 0. \quad (33)$$

This condition provides that $\int_0^\delta dr r |F|^2 < \infty$ for sufficiently small $\delta > 0$.

Analytical properties. To understand the properties of the solution d of Eq. (28), we consider the analytical properties of the coefficients $p(r)$ and $q(r)$, Eqs. (29), (30), on the interval $[0, \infty)$. In the origin, the coefficients behave as $p(r) \sim r^{-1}$, $q(r) \sim r^{-2}$, so that the point $r = 0$ is a regular singular point of the differential equation (28). The coefficient $q(r)$ tends to a constant when $r \rightarrow \infty$, therefore the point $r = \infty$ is an irregular singular point of the equation. The above properties of Eq. (28) (singularities of $p(r)$ and $q(r)$ at $r = 0, \infty$ and boundary condition for $d(r)$ at $r = 0$) are analogous to those of radial Schrödinger equation. The new property of Eq. (28) is the singularity of the coefficient $p(r)$ at $r = r_*(E)$, see Eq. (4), when $E \in (0, V_{\max})$. In principle, the singularities of the coefficients of the equation do not necessarily lead to the singularity of the solution (and its derivatives). One can check that the general solution for $M = 0$ is, indeed, a smooth function at $r = r_*$. Therefore, we concentrate on the case $M \neq 0$. The general solution of Eq. (28) in this case is not smooth at

$r = r_*$, which can be readily seen from the asymptotics of the solution in the vicinity of r_* :

$$d(r) \approx b_1 \left(1 + \frac{M^2 (1 - r/r_*)^2}{2} \ln |1 - r/r_*| \right) + b_2 (1 - r/r_*)^2. \quad (34)$$

Therefore, we search for the solution separately in two regions

$$d(r) = \begin{cases} \tilde{b}_1 d_{\text{irr}}(r) + \tilde{b}_2 d_{\text{reg}}(r), & 0 < r < r_* \\ b_1 d_{\text{irr}}(r) + b_2 d_{\text{reg}}(r) & r_* < r < \infty \end{cases}, \quad (35)$$

where $b_{1,2}$ and $\tilde{b}_{1,2}$ are some constants, and the functions d_{irr} and d_{reg} have the asymptotics

$$d_{\text{irr}}(r) \approx 1 + \frac{M^2 (r_* - r)^2}{2r_*^2} \ln |1 - r/r_*|, \quad (36)$$

$$d_{\text{reg}}(r) \approx \frac{(r_* - r)^2}{r_*^2} \quad (37)$$

at $r \rightarrow r_*$.

Matching conditions at $r = r_$.* In order to determine the general form of the solution of Eq. (28), we need to apply matching conditions at $r = r_*$. Conventional analysis of Eq. (28) in the vicinity of r_* leads to the requirement of the continuity of d and d' at $r = r_*$. Using

these conditions we end up with

$$\tilde{b}_1 = b_1. \quad (38)$$

Note that b_2 remains a free parameter, which means that the function $d(r)$ in the region $r > r_*$ is not entirely determined by that in the region $r < r_*$.

The boundary condition at the origin, Eq. (33), fixes the ratio

$$\tilde{b}_2/\tilde{b}_1 = \beta, \quad (39)$$

where β is the constant which depends on the energy and the form of the potential. Therefore, we have two conditions, (38) and (39), for four constants $b_{1,2}$ and $\tilde{b}_{1,2}$. It means that for any energy in the interval $E \in (0, V_{\text{max}})$ there are two linearly independent solutions which we choose as

$$d_1(r) = b_1 [d_{\text{irr}}(r) + \beta d_{\text{reg}}(r)], \quad (40)$$

$$d_2(r) = b_2 \theta(r - r_*) d_{\text{reg}}(r), \quad (41)$$

where $\theta(x)$ is the Heaviside step function.

Solutions of the system (25)–(27). Let us now return to the initial system, Eqs. (25)–(27). Note that Eqs. (25) and (26) determine functions f and h up to the generalized function localized at $r = r_*$. Substituting (40) and (41) in Eqs. (25)–(27), we obtain two solutions of the equation (24):

$$F_1(E, r) = \begin{pmatrix} \frac{d_1(E, r)}{r} \text{P} \frac{2M}{V(r) - E} \\ \frac{2\partial_r d_1(E, r)}{V(r) - E} \\ d_1(E, r) \end{pmatrix}, \quad (42)$$

$$F_2(E, r) = \begin{pmatrix} \frac{2M d_2(E, r)}{r(V(r) - E)} - \frac{2r \partial_r^2 d_2(E, r_* + 0)}{M} \delta(V(r) - E) \\ \frac{2\partial_r d_2(E, r)}{V(r) - E} \\ d_2(E, r) \end{pmatrix}. \quad (43)$$

Here $\text{P} \frac{1}{x}$ stands for the principal value defined as

$$\text{P} \frac{1}{V(r) - E} = \frac{1}{2} \left(\frac{1}{V(r) - E + i0} + \frac{1}{V(r) - E - i0} \right).$$

In order to check that F_1 and F_2 are the solutions of Eq. (24) in the vicinity of r_* , one can integrate the equations (25)–(27) over r from $r_* - \delta_1$ to $r_* + \delta_2$, and consider the limit $\delta_{1,2} \rightarrow +0$.

Similar to the solutions $g_a(r)$ of the equation (22), the functions $F_{1,2}$ contain generalized functions. The density $\rho = F^\dagger F$, corresponding to the solution F_1 is not integrable at the point $r = r_*$, while that, corresponding to F_2 , is ill-defined. Therefore, for energies in the interval $(0, V_{\text{max}})$ there is no solution $F(E, r)$ of the stationary equation with the density being an integrable function in

the vicinity of $r_*(E)$. This statement is in clear contradiction with the statement of Ref.¹², where it was claimed that nonanalyticities at $r = r_*$ give a finite contribution to the probability.

It may seem that the same consideration of the case $M = 0$ will also lead to the two-fold degeneracy of the spectrum for $0 < E < V_{\text{max}}$. However, it turns out that the substitution of d_2 from Eq. (41) to the original system, Eqs. (25)–(27), leads, for $M = 0$, to appearance of the δ -function term violating Eq. (27).

For completeness, let us also discuss the properties of the solution of Eq. (24) for the energies above the maximum of the potential or below zero. In this case there is no singularity in the coefficient $p(r)$ on the interval $(0, \infty)$. The energy spectrum is not degenerate for $E < 0$

and $E > V_{\max}$ since the solution is defined uniquely (up to the normalization) by the boundary condition at the origin. This solution has the form (42) where one can omit the P symbol. In what follows we assume that $F_1(E, r)$ for $E < 0$ and $E > V_{\max}$ is normalized as

$$\int_0^\infty dr r F_1^\dagger(E, r) F_1(E', r) = 2\pi\delta(E - E'), \quad (44)$$

so that the large- r asymptotics of $F_1(E, r)$ has the form

$$F_1(E, r) \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{r}} \begin{pmatrix} 0 \\ \sin \frac{Er + \varphi}{2} \\ \cos \frac{Er + \varphi}{2} \end{pmatrix}, \quad (45)$$

where φ is some function of the energy.

Alternative derivation. We present now an alternative derivation of the solutions (42) and (43) for $M \neq 0$, which allows one to understand better the appearance of the second solution F_2 . For this purpose we interpret Eq. (24) for real E as a limit of the equation

$$(E + i\epsilon)F = \hat{H}_r F \quad (46)$$

at $\epsilon \rightarrow \pm 0$. The limit depends on the sign of ϵ (see below) and we denote the corresponding solutions by the lower index $+$ or $-$, respectively. The equation for the function $d(r)$ has the form (28) with the replacement $E \rightarrow E + i\epsilon$. For $\epsilon \neq 0$, the coefficient $p(r)$ of this equation has no singularities on the interval $(0, \infty)$ and its solution d_\pm is fixed, up to a constant factor, by the boundary condition at the origin. The first two components of the functions F_\pm can be expressed in terms of d_\pm so that

$$F_\pm(E, r) = \begin{pmatrix} f_\pm(E, r) \\ h_\pm(E, r) \\ d_\pm(E, r) \end{pmatrix} = \begin{pmatrix} \frac{2M d_\pm(E, r)}{r(V(r) - E \mp i0)} \\ \frac{2\partial_r d_\pm(E, r)}{V(r) - E \mp i0} \\ d_\pm(E, r) \end{pmatrix}, \quad (47)$$

where we assume that the limit $\epsilon \rightarrow \pm 0$ is already performed. On the interval $(0, r_*(E))$ the functions F_+ and F_- coincide. Without loss of generality, we can choose them to be real on this interval. Then, obviously, $F_+(E, r) = F_-^*(E, r)$ on the whole interval $(0, \infty)$. On the interval $(r_*(E), \infty)$ the functions F_\pm gain imaginary parts which is clearly seen from the asymptotics of the functions d_\pm in the vicinity of r_* :

$$\begin{aligned} d_\pm(E, r) &\approx b_1 \left(1 + \frac{M^2(1 - r/r_*)^2}{2} \ln \left(\frac{V(r) - E \mp i0}{|V'(r_*)| r_*} \right) + \beta(1 - r/r_*)^2 \right) \\ &\approx b_1 \left(1 + \frac{M^2(1 - r/r_*)^2}{2} \ln \left(\frac{r_* - r}{r_*} \mp i0 \right) + \beta(1 - r/r_*)^2 \right). \end{aligned} \quad (48)$$

The prescription $\pm i0$ determines the choice of the logarithm branch for $r > r_*$, so that

$$d_\pm(E, r) \approx b_1 \left(1 + \frac{M^2(1 - r/r_*)^2}{2} \ln \left| \frac{r_* - r}{r_*} \right| + \left(\beta \mp i \frac{\pi M^2}{2} \theta(r - r_*) \right) (1 - r/r_*)^2 \right). \quad (49)$$

Using this formula, as well as the identity

$$\frac{1}{V(r) - E \mp i0} = P \frac{1}{V(r) - E} \pm i\pi\delta(V(r) - E), \quad (50)$$

one can check that the real part of F_\pm is proportional to the function F_1 , Eq. (42), and the imaginary part of F_\pm is proportional to the function F_2 , Eq. (43).

Orthonormality and the dual basis. For the potential decreasing faster than $1/r$, the asymptotics of the functions d_\pm at $r \rightarrow \infty$ has the form

$$d_\pm(E, r) \rightarrow \frac{c}{2\sqrt{r}} \left(e^{\mp i(Er + \varphi)/2} + \gamma e^{\pm i(Er + \varphi)/2} \right), \quad (51)$$

where c , γ , and φ are, in general, some real-valued functions of the energy. For the potential decreasing at $r \rightarrow \infty$ as α/r , one should perform the replacement $\varphi \rightarrow \varphi - \alpha \ln Er$. We choose the overall normalization constant c to be equal to unity, so that the asymptotics of the functions F_\pm has the form

$$F_\pm(E, r) \rightarrow \frac{1}{2\sqrt{r}} \left[\begin{pmatrix} 0 \\ \pm i \\ 1 \end{pmatrix} e^{\mp i(Er + \varphi)/2} + \gamma \begin{pmatrix} 0 \\ \mp i \\ 1 \end{pmatrix} e^{\pm i(Er + \varphi)/2} \right]. \quad (52)$$

Then the functions F_{\pm} satisfy the relation

$$\int_0^{\infty} dr r F_{\sigma}^{\dagger}(E, r) F_{\sigma'}(E', r) = 2\pi\delta(E - E') N_{\sigma\sigma'}, \quad (53)$$

$$N_{++} = N_{--} = \frac{1 + \gamma^2}{2} + \frac{4\pi M^2 |b_1|^2}{r^{\star} |V'(r_{\star})|}, \quad (54)$$

$$N_{+-} = N_{-+} = \gamma, \quad (55)$$

where $b_1 = d_{\pm}(E, r_{\star})$, see Eq. (49). There is one subtle relation between constants b_1 and γ , which follows from the conservation of the total radial current $J_r(r) = 2\pi r j_r$, where j_r is defined in Eq. (20). Namely, using the equality $J_r(r \rightarrow r_{\star} + 0) = J_r(r \rightarrow \infty)$, we obtain

$$\frac{4\pi M^2 |b_1|^2}{r^{\star} |V'(r_{\star})|} = \frac{1 - \gamma^2}{2}, \quad (56)$$

so that

$$N_{++} = N_{--} = 1. \quad (57)$$

Note that $J_r \neq 0$ in the region $r > r_{\star}$. The existence of the solutions with the nonzero radial current is the consequence of the spectrum degeneracy. For $r < r_{\star}$ we have $J_r = 0$. It may seem that such a behaviour contradicts the continuity equation at $r = r_{\star}$. However, the density $\rho = F^{\dagger}F$ is ill-defined at $r = r_{\star}$, so it does not make sense to consider the continuity condition for j_r at this point.

Since the wave functions $F_{\pm}(E, r)$ are not orthogonal to each other, it is convenient to introduce the dual basis functions $G_{\pm}(E, r)$ being the linear combinations of $F_{\pm}(E, r)$ and satisfying the relations:

$$\int_0^{\infty} dr r G_{\sigma}^{\dagger}(E, r) F_{\sigma'}(E', r) = 2\pi\delta(E - E') \delta_{\sigma\sigma'}. \quad (58)$$

From Eqs. (53), (57) we have

$$G_{\pm}(E, r) = \frac{F_{\pm} - \gamma F_{\mp}}{1 - \gamma^2}. \quad (59)$$

Using Eq. (52), we find that the large-distance asymptotics of G_{\pm} corresponds to the convergent/divergent spherical wave, respectively:

$$G_{\pm}(E, r) \rightarrow \frac{e^{\mp i(Er + \varphi)/2}}{2\sqrt{r}} \begin{pmatrix} 0 \\ \pm i \\ 1 \end{pmatrix}. \quad (60)$$

This remarkable property is important in the consideration of the time-dependent problem.

IV. TIME-DEPENDENT PROBLEM

The stationary solutions for $M \neq 0$, derived in the previous section, look very unusual due to a singular behaviour at $r = r_{\star}$. This behaviour should be reflected in

the time evolution of wave packets. Note that Eq. (16) has the form resolved with respect to the derivative $\partial_t F$. Besides, the coefficients of the differential operator \hat{H}_r in the right-hand side are smooth functions on the interval $(0, \infty)$. So, for suitable initial and boundary conditions, the problem of finding the solution $F(t, r)$ is well-posed.

We choose the initial conditions as

$$F(0, r) = \frac{C}{\sqrt{r}} \begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix} e^{-i\frac{E_0 r}{2}} \Omega\left(\frac{r - r_0}{\Delta}\right), \quad (61)$$

$$\Omega(x) = (1 - x^2)^2 \theta(1 - x^2), \quad (62)$$

where C is the normalization constant, determined by the relation $\int_0^{\infty} dr r |F|^2 = 1$. This form corresponds to the scattering problem setup and describes the wave packet with the average energy E_0 and the width Δ , moving from the large distance r_0 towards the origin (cf. Eq. (52)). We assume that $r_0 \gg \Delta \gg |E_0|^{-1}$, i.e., the packet width in the coordinate space is small compared to the average value of r , and the width in the momentum space is small compared to the average value of E . If the potential $V(r)$ is a localized function falling off at $r \sim R$, then we also assume that $\Delta \gg R$. Performing the numerical integration of Eq. (16) over t , we find $F(t, r)$. The initial packet with the energy E_0 well above V_{\max} (when $E_0 - V_{\max} \gg 1/\Delta$) or well below zero ($-E_0 \gg 1/\Delta$) moves with the speed $2v_F$ (2 in our units), comes to small distances, reflects, and goes away. The norm of the outgoing packet is the same as that of the incoming one. This behaviour looks very similar to that of the wave packet obeying the massless Dirac equation in the central external field. The evolution of the wave packet with the energy E_0 deep inside the interval $(0, V_{\max})$ is essentially different. During the scattering process a narrow peak develops at $r_{\star}(E_0)$. The form of the peak stabilizes at large time. The norm of the outgoing packet (corresponding to the reflected particles) is less than that of the incoming one. However, the total norm is conserved due to the additional contribution of the peak at finite distances (corresponding to the “adhered” particles). To demonstrate this behaviour, the time evolution of the wave packet (61) in the Coulomb potential $V(r) = \alpha/r$ is shown in Fig. 1. One can see that, after reflection, a narrow peak appears at $r_{\star} = \alpha/E_0$.

Decomposition method. In order to gain deeper insight into this behaviour, let us derive the time evolution of the wave packet using the decomposition of the initial wave packet over the stationary wave functions. The decomposition has the form

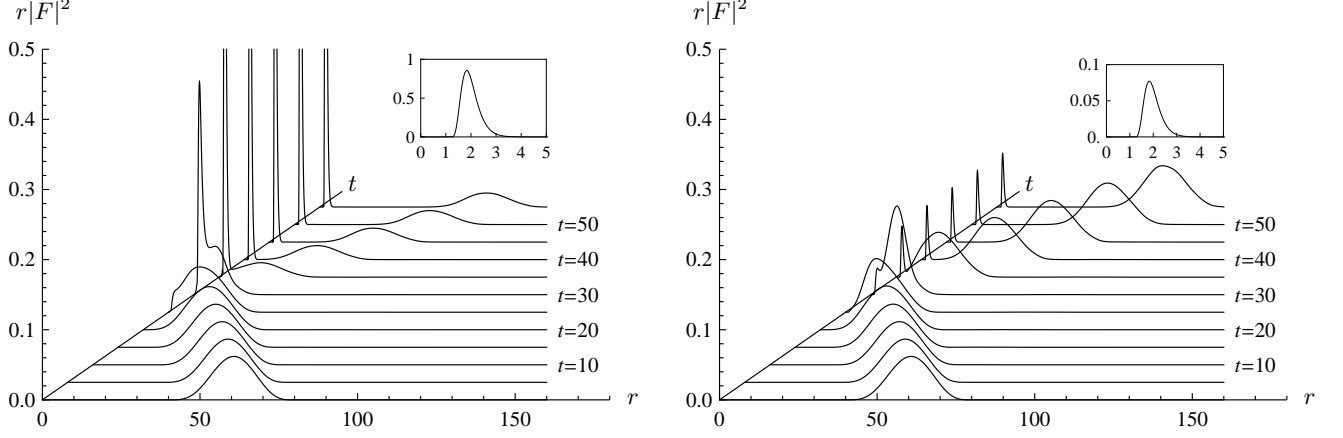


Figure 1: Time evolution of the density, corresponding to the wave packet (61), in the Coulomb potential $V(r) = \alpha/r$. The parameters are , $E_0 = 1$, $r_0 = 60$, $\Delta = 20$, $\alpha = 2$, $M = 1$ (left) and $M = 2$ (right). Insets: the form of the peak at large time.

$$\begin{aligned}
 F(t, r) = & \int_0^{V_{\max}} \frac{dE}{2\pi} e^{-iEt} [C_+(E) F_+(E, r) + C_-(E) F_-(E, r)] \\
 & + \int_{-\infty}^0 \frac{dE}{2\pi} C(E) e^{-iEt} F_1(E, r) + \int_{V_{\max}}^{\infty} \frac{dE}{2\pi} C(E) e^{-iEt} F_1(E, r) .
 \end{aligned} \tag{63}$$

The coefficients $C(E)$ and $C_{\pm}(E)$ have the form

$$C(E) = \int_0^{\infty} dr r F_1^{\dagger}(E, r) F(0, r), \tag{64}$$

$$C_{\pm}(E) = \int_0^{\infty} dr r G_{\pm}^{\dagger}(E, r) F(0, r). \tag{65}$$

Note that the coefficients $C_{\pm}(E)$ in front of $F_{\pm}(E, r)$ in the decomposition (63) are expressed via the overlap integrals of $F(0, r)$ with the elements $G_{\pm}^{\dagger}(E, r)$ of the

dual basis. Let us consider the decomposition of the wave packet (61) with the energy E_0 deep inside the interval $(0, V_{\max})$, when $V_{\max} - E_0 \gg 1/\Delta$ and $E_0 \gg 1/\Delta$. In this case the main contribution to the integrals in Eqs. (64) and (65) comes from large distances $r \sim r_0$. Therefore, for the calculation of the coefficients $C(E)$ and $C_{\pm}(E)$, we can use the large- r asymptotics (45) and (52). We obtain that $C(E)$ and $C_-(E)$ are suppressed due to the fast oscillations of the integrands, and we can omit the corresponding contributions in Eq. (63). The coefficient $C_+(E)$ has the form

$$C_+(E) = \tilde{C}(E) \exp(iEr_0/2) \tilde{\Omega}\left(\frac{(E - E_0)\Delta}{2}\right), \tag{66}$$

$$\tilde{\Omega}(q) = \int dx \exp(iqx) \Omega(x) = \frac{16}{q^5} [(3 - q^2) \sin q - 3q \cos q], \tag{67}$$

$$\tilde{C}(E) = \frac{\sqrt{\Delta/2}}{\sqrt{\int dx \Omega^2(x)}} e^{-i(E_0 r_0 - \varphi(E))/2} = \sqrt{\frac{315\Delta}{512}} e^{-i(E_0 r_0 - \varphi(E))/2}. \tag{68}$$

The function $\tilde{\Omega}\left(\frac{(E - E_0)\Delta}{2}\right)$ is peaked around $E = E_0$ with the characteristic width $1/\Delta$, while $\tilde{C}(E)$ is some

slowly varying function of the energy. Therefore, we can

represent the function $F(t, r)$ as

$$F(t, r) = \tilde{C}(E_0) \int_0^{V_{\max}} \frac{dE}{2\pi} e^{-iE\tau} \tilde{\Omega}\left(\frac{(E - E_0)\Delta}{2}\right) F_+(E, r), \quad (69)$$

where $\tau = t - r_0/2$.

Let us demonstrate now that this decomposition leads to the appearance of the peak in the vicinity of $r = r_*(E_0)$ at large t . For this purpose we consider the

asymptotic form of $F(t, r)$ for t satisfying the condition $|2t - r_0| \gg \Delta$ and for r obeying the condition $r_*|V'(r_*)||r - r_*| \ll 1$. Keeping in $F_+(E, r)$, Eq. (47), only the singular component

$$f_+(E, r) = \frac{2Md_+(E, r)}{r(V(r) - E - i0)}, \quad (70)$$

and using the identity (50), we obtain

$$f(t, r) \approx \frac{2M\tilde{C}(E_0)}{r} \int_0^{V_{\max}} \frac{dE}{2\pi} e^{-iE\tau} \tilde{\Omega}\left(\frac{(E - E_0)\Delta}{2}\right) \left(P \frac{1}{V - E} + i\pi\delta(V - E)\right) d_+(E, r), \quad (71)$$

where $V = V(r)$. Passing to the variable $\varepsilon = E - V$ we have

$$f(t, r) \approx \frac{2M\tilde{C}(E_0)}{r} e^{-iV\tau} \int_{L_1}^{L_2} \frac{d\varepsilon}{2\pi} e^{-i\tau\varepsilon} \tilde{\Omega}\left(\frac{\Delta(V - E_0 + \varepsilon)}{2}\right) \left(i\pi\delta(\varepsilon) - P \frac{1}{\varepsilon}\right) d_+(V + \varepsilon, r), \quad (72)$$

where $L_1 = -V$, $L_2 = V_{\max} - V$. Since $|\tau| \gg \Delta$ and $|\tau L_{1,2}| \gg 1$, we can write Eq. (72) as

$$f(t, r) \approx \frac{2M\tilde{C}(E_0)}{r} e^{-iV\tau} \tilde{\Omega}\left(\frac{\Delta(V - E_0)}{2}\right) d_+(V, r) \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} e^{-i\tau\varepsilon} \left(i\pi\delta(\varepsilon) - P \frac{1}{\varepsilon}\right). \quad (73)$$

The remaining integral is equal to $i\theta(\tau)$, and finally we come to the asymptotics of $f(t, r)$ at $|\tau| = |t - r_0/2| \gg \Delta$:

$$f(t, r) \approx \frac{2iM\tilde{C}(E_0)}{r} e^{-iV\tau} \tilde{\Omega}\left(\frac{\Delta(V - E_0)}{2}\right) d_+(V, r) \theta(\tau). \quad (74)$$

Note that the right-hand side of Eq. (74) vanishes for $\tau \ll -\Delta$, and the leading asymptotics of $F(t, r)$ comes from the contribution of the nonsingular terms. However, we can claim that this asymptotics is not peaked in the vicinity of $r_*(E_0)$. For $\tau \gg \Delta$, the density $|F|^2 \approx |f|^2$ is independent of τ and peaked, due to the factor $\tilde{\Omega}$ in Eq. (74), with the characteristic width $\delta \sim 1/|V'(r_*)\Delta|$. Thus, we have demonstrated that the decomposition method leads to the appearance of the peak at large time, which is in agreement with the result of direct numerical solution of the differential equation. For the Coulomb potential, we have also checked numerically that the time evolution, obtained by the decomposition method, coincides with that obtained by the direct numerical solution of the differential equation, see Fig. 1.

Adhesion coefficient. Let us consider the quantity

$$A = \lim_{t \rightarrow +\infty} \int_0^L dr r |F(t, r)|^2. \quad (75)$$

The upper limit L in this formula is some fixed parameter obeying the condition $L \gg r_*(E_0)$. The quantity A is the adhesion coefficient, i.e., the probability for the two particles to remain at finite distances at large t . Using Eqs. (74), (67), (68), (49), and (56) we obtain

$$A \approx \lim_{t \rightarrow +\infty} \int_0^L dr r |f(t, r)|^2 \approx 1 - \gamma^2, \quad (76)$$

where $\gamma = \gamma(E_0)$. For the Coulomb potential $V(r) = \alpha/r$, the dimensional arguments lead to the independence of the quantity γ of $|E_0|$. In Fig. 2 the adhesion coefficient A for the case of Coulomb potential is shown as a function of α . One can see that A grows when α changes from 0 to its critical value $\alpha_M = \sqrt{1 + 4M^2}$ (when the parameter ν in Eq. (32) vanishes).

Asymptotically localized state. The numerical solution of the differential equation (16) shows that at large t and fixed r the functions $h(t, r)$ and $d(t, r)$ vanish. Then, it follows from Eq. (13) that $f(t, r) \xrightarrow{t \rightarrow \infty} e^{-iV(r)t} f_0(r)$,

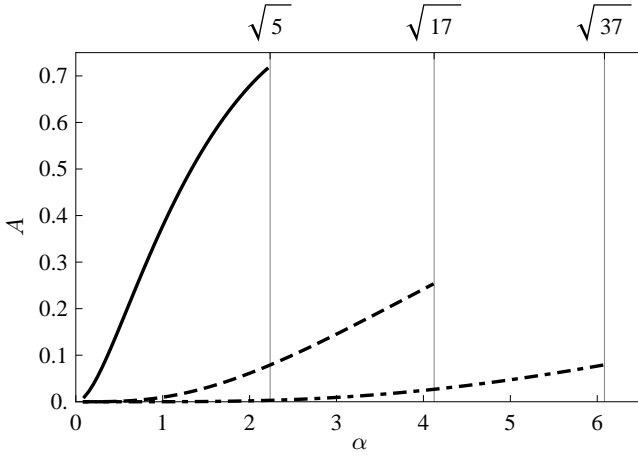


Figure 2: The adhesion coefficient A , Eq. (76), in the Coulomb potential as a function of α for $M = 1$ (solid curve), $M = 2$ (dashed curve), $M = 3$ (dash-dotted curve). The vertical lines correspond to the critical values $\alpha_M = \sqrt{1 + 4M^2}$.

where $f_0(r)$ is some function of r . This form of the asymptotics is also in agreement with Eq. (74). The function $f_0(r)$ is peaked at $r = r_*$ and depends on the form of the initial packet (61). This asymptotics could be considered as a hint for the existence of the normalizable solutions of Eq. (16) with the constant density $\rho(r) = |f_0(r)|^2$. However, the equation (16) has no solutions of the form

$$F(t, r) = e^{-iV(r)t} \begin{pmatrix} f_0(r) \\ 0 \\ 0 \end{pmatrix}.$$

Indeed, this form satisfies Eqs. (13) and (14), but not (15). Instead, we search the asymptotics of the solution of Eqs. (13)-(15) as

$$F(t, r) = e^{-iV(r)t} \sum_{n=0}^{\infty} \begin{pmatrix} f_n(r) \\ h_n(r) \\ d_n(r) \end{pmatrix} t^{-n}. \quad (77)$$

Substituting this form in Eq. (16), we obtain the recurrence relations for $f_n(r)$, $h_n(r)$, and $d_n(r)$ which can be used to express the asymptotics (77) via one function $f_0(r)$. In the leading order we obtain

$$f(t, r) = e^{-iV(r)t} [f_0(r) + O(t^{-2})], \quad (78)$$

$$h(t, r) = \frac{e^{-iV(r)t}}{t} \left[\frac{iM f_0(r)}{rV'(r)} + O(t^{-1}) \right], \quad (79)$$

$$d(t, r) = \frac{e^{-iV(r)t}}{t^3} \left[-\frac{iM f_0(r)}{2rV'^2(r)} + O(t^{-1}) \right]. \quad (80)$$

Though the function $h(t, r)$ vanishes at $t \rightarrow \infty$, its derivative $\partial_r h(t, r)$ does not vanish, $|\partial_r h(t, r)| \rightarrow |M f(r)/r|$. Due to this behaviour of $h(t, r)$, the equation (15) is now satisfied. We see that the asymptotics

(78)-(80) is in agreement with the behaviour observed in the numerical solution of the differential equation. Note that the asymptotics (78)-(80) leads to the vanishing radial and azimuthal current, Eq. (20).

V. CONCLUSION

In the present paper, we have considered a model of the electron-electron interaction in graphene, based on the hamiltonian (3). Despite the simplicity of the model, it leads to a very unusual dynamics. We have shown, both numerically and analytically, that in the process of the wave packet scattering the asymptotically localized state appears, see Fig. (1) and Eq. (74). From the point of view of the outside observer, the scattering seems to be inelastic. The origin of this phenomenon is traced back to two-fold degeneracy of the spectrum of hamiltonian H_r , Eq. (17), at $0 < E < V_{\max}$, Eqs. (42) and (43). This degeneracy is related to the degeneracy of the derivative matrix in \hat{H}_r . The results obtained are valid for any smooth monotonically decreasing vanishing potential. Though we did not take into account the Fermi statistics of the interacting electrons, the requirement of the Fermi statistics can be satisfied by appropriate choice of the spin part of the wave function.

For simplicity, we considered the states with definite value of J^z . It is obvious, that the observed phenomenon (the appearance of the asymptotically localized state) also retains for any superposition of the states with different values of J^z . Our consideration is not directly applicable to the case $\mathbf{P} \neq 0$, but the appearance of the asymptotically localized state is likely to take place also in this case because the derivative matrix in H_V , Eq. (3), is also degenerate.

We emphasize that this simple model does not take into account the existence of the electrons below Fermi surface. The effect of such electrons is the appearance of virtual electron-hole pairs in the intermediate states. While the exact account of this effect is hardly possible, its qualitative consideration is very important and will be presented elsewhere. It seems that the effect of the electrons below Fermi surface is small at least in the case when $\delta E_F < 0$ and $|\delta E_F| \gg E_0$, where δE_F is the difference between the Fermi energy and the energy of the Dirac point. Therefore, it should be possible to observe the appearance of the asymptotically localized state in the experiment. Note that the differential equation (5) does not take into account the effect of the finite lattice scale $l_0 \sim 0.14\text{nm}$, and valid if the wave function changes slowly on this scale. It gives us two conditions: the width of the localized state should be much larger than the lattice scale, and the variation of the phase on the lattice scale should be small compared to unity. The first condition gives the constraint on the energy dispersion δE in the wave packet:

$$\delta E \gg |V'(r_*)| l_0.$$

It follows from Eq. (74) that, at large time, the phase of the wave function varies significantly on the lattice scale. The second condition gives us the lower bound τ_0 of the life time of the localized state:

$$\tau_0 \sim \frac{1}{l_0 |V'(r_*)|} \gg 1/\delta E,$$

which means that the localized state lives long enough. For the Coulomb potential, these two conditions read

$$\begin{aligned} \delta E &\gg \frac{E_0^2 l_0}{\alpha}, \\ \tau_0 &\sim \frac{\alpha}{l_0 E_0^2}. \end{aligned}$$

Note that the first condition is compatible with the condition $\delta E \ll E_0$ provided that E_0 is sufficiently small. For instance, for $E_0 \sim 1\text{meV}$ and $\alpha \sim 1$, we have quite large time $\tau_0 \sim 1\mu\text{s}$. Therefore, if the model considered is relevant to the electron-electron interaction in graphene, one may hope to observe the long-lived localized states in the experiment.

Acknowledgements This work was supported by Federal special-purpose program “Scientific and scientific-pedagogical personnel of innovative Russia”, RFBR grant No. 11-02-00220. The work of I.S.T. was also supported by the “Dynasty” foundation.

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